Supporting Information:

Role of solvation dynamics and local ordering of water in inducing conformational transitions in Poly(N-isopropylacrylamide) oligomers through the LCST

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Table S1: PCFF parameters for water model

Quartic polynomial for bond stretching				
Bonds	b_0 (Å)	K_2 (Kcal.mol^{-1}. Å^{-2})	K_3 (Kcal.mol^{-1}. Å^{-3})	K_4 (Kcal.mol^{-1}. Å^{-4})
O-H	0.9700	563.2800	-1428.2200	1902.1200

Quartic polynomial for angle bending				
Bond angles	θ_0 (degrees)	H_2 (Kcal.mol^{-1}. deg^{-2})	H_3(Kcal.mol^{-1}.deg^{-3})	H_4(Kcal.mol^{-1}. Deg^{-4})
H-O-H	0.9700	49.8400	-11.6000	-8.000

Non-bonded Van der Waals interactions		
Bond angles	σ (Å)	ε (Kcal.mol^{-1})
O	3.6080	0.27400
H	1.0980	0.1300

The decay time for both residence time ($P_{res}(t)$) and hydrogen bond correlations were defined as the time it takes to reach 37% of the initial value. In this case, the correlation functions are normalized and hence the decay time is the time taken to reach a value of 0.37. Table 2, 3, 4, and 5 show the decay time for $P_{res}(t)$ and hydrogen bond correlation.

Table S2: Decay time for residence probability.

System	278 K		310 K	
	Decay time (ps)	Standard deviation	Decay time (ps)	Standard deviation
3-mer	~6	0.21	~5	0.25
5-mer	~9	0.19	~6	0.22
10-mer	~14	0.17	~8	0.19
30-mer	~17	0.17	~11	0.18

Table S3: Decay time for hydrogen bond correlation function for polymer-polymer (Type 1) hydrogen bonds.

System	278 K		310 K	
	Decay time (ps)	Standard deviation	Decay time (ps)	Standard deviation
3-mer	~4	0.26	~1	0.42
5-mer	~6	0.21	~7	0.19
10-mer	~17	0.13	~5	0.19
30-mer	~4	0.25	> 37	-

Table S4: Decay time for hydrogen bond correlation function for polymer-water (Type 2) hydrogen bonds.

System	278 K		310 K	
	Decay time (ps)	Standard deviation	Decay time (ps)	Standard deviation
3-mer	~4	0.25	~2	0.31
5-mer	~5	0.23	~3	0.28
10-mer	~5	0.24	~2	0.36
30-mer	~10	0.18	~5	0.22

Table S5: Decay time for hydrogen bond correlation function for water- polymer (Type 3) hydrogen bonds.

System	278 K		310 K	
	Decay time (ps)	Standard deviation	Decay time (ps)	Standard deviation
3-mer	~1	0.41	~1	0.48
5-mer	~1	0.39	~1	0.46
10-mer	~2	0.37	~1	0.43
30-mer	~2	0.36	~1	0.38